CLAIMS

what is claimed is:

1. A method of predicting whether an organic compound will penetrate the blood brain barrier significantly, the method comprising:

(a) determining whether the compound has fewer than six hydrogen bond donors and hydrogen bond acceptors; and

(b) based on whether the compound has fewer than six hydrogen bond donors and hydrogen bond acceptors, predicting whether the compound will penetrate the blood brain barrier significantly, wherein the compound is predicted to penetrate the blood brain barrier significantly only if it has fewer than six hydrogen bond donors and hydrogen bond acceptors.

2. The method of claim 1, wherein the method is implemented on a computing device.

3. The method of claim 2, further comprising:

receiving a representation of the compound; and

analyzing the compound in a manner that automatically identifies hydrogen bond donors and hydrogen bond acceptors.

4. The method of claim 2, further comprising redesigning the compound by adding one or more hydrogen bond donors and/or hydrogen bond acceptors, wherein the compound originally had fewer than six total hydrogen bond donors and hydrogen bond acceptors and now has six or more total hydrogen bond donors and hydrogen bond acceptors.

5. The method of claim 2, further comprising redesigning the compound by removing one or more hydrogen bond donors and/or hydrogen bond acceptors wherein the compound originally had six or more total hydrogen bond donors and hydrogen bond acceptors and now has fewer than six total hydrogen bond donors and hydrogen bond acceptors.

6. The method of claim 2, further comprising automatically repeating (a) and (b) for multiple different compounds.

7. A computer program product comprising a machine-readable medium on which are provided program instructions for predicting whether an organic compound will penetrate the blood brain barrier significantly, the instructions comprising:

(a) determining whether the compound has fewer than six hydrogen bond donors and hydrogen bond acceptors; and

(b) based on whether the compound has fewer than six hydrogen bond donors and hydrogen bond acceptors, predicting whether the compound will penetrate the blood brain barrier significantly, wherein the compound is predicted to penetrate the blood brain barrier significantly only if it has fewer than six hydrogen bond donors and hydrogen bond acceptors.

8. The computer program product of claim 7, wherein the program instructions further comprise:

receiving a representation of the compound; and analyzing the compound in a manner that automatically identifies hydrogen bond donors and hydrogen bond acceptors.

9. The computer program product of claim 7, wherein the program instructions further comprise:

redesigning the compound by adding one or more hydrogen bond donors and/or hydrogen bond acceptors, wherein the compound originally had fewer than six total hydrogen bond donors and hydrogen bond acceptors and now has six or more total hydrogen bond donors and hydrogen bond acceptors.

10. The computer program product of claim 7, wherein the program instructions comprise:

redesigning the compound by removing one or more hydrogen bond donors and/or hydrogen bond acceptors wherein the compound originally had six or more total hydrogen bond donors and hydrogen bond acceptors and now has fewer than six total hydrogen bond donors and hydrogen bond acceptors.

11. The computer program product of claim 7, further comprising program instructions for automatically repeating (a) and (b) for multiple different compounds.

12. An apparatus for predicting whether an organic compound will penetrate the blood brain barrier significantly, the apparatus comprising:

(a) an interface for receiving representations of organic compounds;

(b) a memory coupled for communication with said interface; and

(c) a processor coupled for communication with said memory, wherein at least one of the memory and the processor includes logic for: (i) determining whether the compound has fewer than six hydrogen bond donors and hydrogen bond acceptors; and (ii) based on whether the compound has fewer than six hydrogen bond donors and hydrogen bond acceptors, predicting whether the compound will penetrate the blood brain barrier significantly, wherein the compound is predicted to penetrate the blood brain barrier significantly only if it has fewer than six hydrogen bond donors and hydrogen bond acceptors.

13. A method of analyzing a compound, the method comprising:

(a) determining a total number of hydrogen bond donors and hydrogen bond acceptors on the compound;

(b) determining a partitioning property of the compound;

(c) based on at least the total number of hydrogen bond donors and hydrogen bond acceptors, classifying the compound based upon its ability to penetrate the blood brain barrier; and

(d) based upon the total number of hydrogen bond donors and hydrogen bond acceptors and the partitioning property, classifying the compound according to at least one of (i) its solubility and (ii) its ability to be absorbed in the intestine.

14. The method of claim 13, wherein the compound is classified based on both its solubility and its ability to be absorbed in the intestine.

15. The method of claim 13, wherein the classifying of (d) is performed by determining where the compound lies with respect to a line or curve defining a transition between solubility/insolubility or absorption/non-absorption in the intestine, wherein the line or curve bisects a two-dimensional space of hydrogen bond donor and acceptor count versus partitioning property.

16. The method of claim 13, wherein (c) and (d) employ a model comprising:

a two-dimensional space of hydrogen bond donor and acceptor count versus partitioning property, and

a first line through said two-dimensional space, which first line separates a first region containing compounds that substantially penetrate the blood brain barrier from a second region containing compounds that do not substantially penetrate the blood brain

barrier, and wherein the first line is substantially perpendicular to an axis specifying the total number of hydrogen bond donors and hydrogen bond acceptors in the two-dimensional space.

17. The method of claim 16, wherein the first line crosses the axis at a value of about six total hydrogen bond donors and hydrogen bond acceptors.

18. The method of claim 13, wherein the method is implemented on a computer.

19. A computer program product comprising a machine readable medium on which is provided program instructions for analyzing compounds, the program instructions specifying at least the following operations:

(a) determining a total number of hydrogen bond donors and hydrogen bond acceptors on a compound;

(b) determining a partitioning property of the compound;

(c) based on at least the total number of hydrogen bond donors and hydrogen bond acceptors, classifying the compound based upon its ability to cross the blood brain barrier; and

(d) based upon the total number of hydrogen bond donors and hydrogen bond acceptors and the partitioning property, classifying the compound according to at least one of (i) its solubility and (ii) its ability to be absorbed in the intestine.

20. The computer product of claim 19, wherein the program instructions specifying (d) classifies the compound based on both its solubility and its ability to be absorbed in the intestine.

21. The computer program product of claim 19, wherein the classifying of (d) is performed by determining where the compound lies with respect to a line or curve defining a transition between solubility/insolubility or absorption/non-absorption in the intestine, wherein the line or curve bisects a two-dimensional space of hydrogen bond donor and acceptor count versus partitioning property.

22. The computer program product of claim 19, wherein (c) and (d) employ a model comprising:

a two-dimensional space of hydrogen bond donor and acceptor count versus partitioning property, and

a first line through said two-dimensional space, which first line separates a first region containing compounds that substantially penetrate the blood brain barrier from a second region containing compounds that do not substantially penetrate the blood brain barrier, and wherein the first line is substantially perpendicular to an axis specifying the total number of hydrogen bond donors and hydrogen bond acceptors in the two-dimensional space.

23. The computer program product of claim 22, wherein the first line crosses the axis at a value of about six total hydrogen bond donors and hydrogen bond acceptors.

24. A machine readable medium on which is provided at least a representation of a two-dimensional space defined by a first axis over which a partitioning property of chemical compounds varies and a second axis over which the sum of hydrogen bond donors and hydrogen bond acceptors of chemical compounds varies,

wherein the two-dimensional space is divided into a first region defining compounds predicted to significantly cross the blood brain barrier and a second region defining compounds predicted to not significantly cross the blood brain barrier and a second region defining compounds predicted to not significantly cross the blood brain barrier and a second region defining compounds predicted to not significantly cross the blood brain barrier.

25. The machine-readable medium of claim 24, wherein the first and second regions are separated by a first line or curve that is substantially perpendicular to the second axis.

26. The machine readable medium of claim 25, wherein the first line crosses the second axis at about a value of six hydrogen bond donors and hydrogen bond acceptors.

27. The machine readable medium of claim 24, wherein the two-dimensional space is further divided into a third region defining compounds predicted to have a solubility greater than a defined value and a fourth region defining compounds predicted to have a solubility lower than the defined value, wherein the third and fourth regions overlap the first and second regions.

28. The machine readable medium of claim 27, wherein the two-dimensional space is further divided into a fifth region defining compounds predicted to have an absorption in the intestine of greater than a second defined value and a sixth region

defining compound predicted to have an absorption in intestine of less than the second defined value, wherein the first and second regions overlap the fifth region.

29. The machine readable medium of claim 27, wherein the third region comprises a first sub-region defining compounds predicted to have a solubility of less than a second predefined value and a second sub-region defining compounds predicted to have a solubility greater than the second defined value.

30. The machine readable medium of claim 24, wherein the two-dimensional space is further divided into a third region defining compounds predicted to have an absorption in the intestine of greater than a defined value and a fourth region defining compounds predicted to have an absorption in the intestine of less than the defined value, wherein the third region overlaps with the first and second regions.

31. The machine readable medium of claim 30, wherein the third region comprises a first sub-region defining compounds predicted to have an absorption in the intestine of less than a second defined value and a second sub-region defining compounds predicted to have an absorption in the intestine of greater than the second defined value.

32. An apparatus for analyzing compounds to predict one or more medicinal properties, the apparatus comprising:

(a) an interface for receiving representations of chemical compounds;

(b) a memory coupled for communication with the interface; and

(c) a processor coupled for communication with said memory, wherein at least one of the memory and the processor contains logic for determining where a given compound resides in a two-dimensional space,

wherein the two-dimensional space is defined by a first axis over which a partitioning property of chemical compounds varies and a second axis over which the sum of hydrogen bond donors and hydrogen bond acceptors of chemical compounds varies, and

wherein a representation of the two-dimensional space employed by the apparatus is divided into a first region defining compounds predicted to significantly cross the blood brain barrier and second region defining compounds predicted to not significantly cross the blood brain barrier.

33. The apparatus of claim 32, wherein the first and second regions are separated by a first line or curve that is substantially perpendicular to the second axis.

34. The computer readable medium of claim 33, wherein the first line crosses the second axis at about a value of six hydrogen bond donors and hydrogen bond acceptors.

35. The apparatus of claim 32, wherein the two-dimensional space is further divided into a third region defining compounds predicted to have a solubility greater than a defined value and a fourth region defining compounds predicted to have a solubility lower than the defined value, wherein the third and fourth regions overlap the first and second regions.

36. The apparatus of claim 35, wherein the two-dimensional space is further divided into a fifth region defining compounds predicted to have an absorption in the intestine of greater than a second defined value and a sixth region defining compound predicted to have an absorption in intestine of less than the second defined value, wherein the first and second regions overlap the fifth region.

37. The apparatus of claim 35, wherein the third region comprises a first sub-region defining compounds predicted to have a solubility of less than a second predefined value and a second sub-region defining compounds predicted to have a solubility greater than the second defined value.

38. The apparatus of claim 32, wherein the two-dimensional space is further divided into a third region defining compounds predicted to have an absorption in the intestine of greater than a defined value and a fourth region defining compounds predicted to have an absorption in the intestine of less than the defined value, wherein the third region overlaps with the first and second regions.

39. The apparatus of claim 38, wherein the third region comprises a first sub-region defining compounds predicted to have an absorption in the intestine of less than a second defined value and a second sub-region defining compounds predicted to have an absorption in the intestine of greater than the second defined value.